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Long Route or Short Cut? A Molecular Dynamics Study of Traffic of Thiocholine within the Active-site Gorge of Acetylcholinesterase

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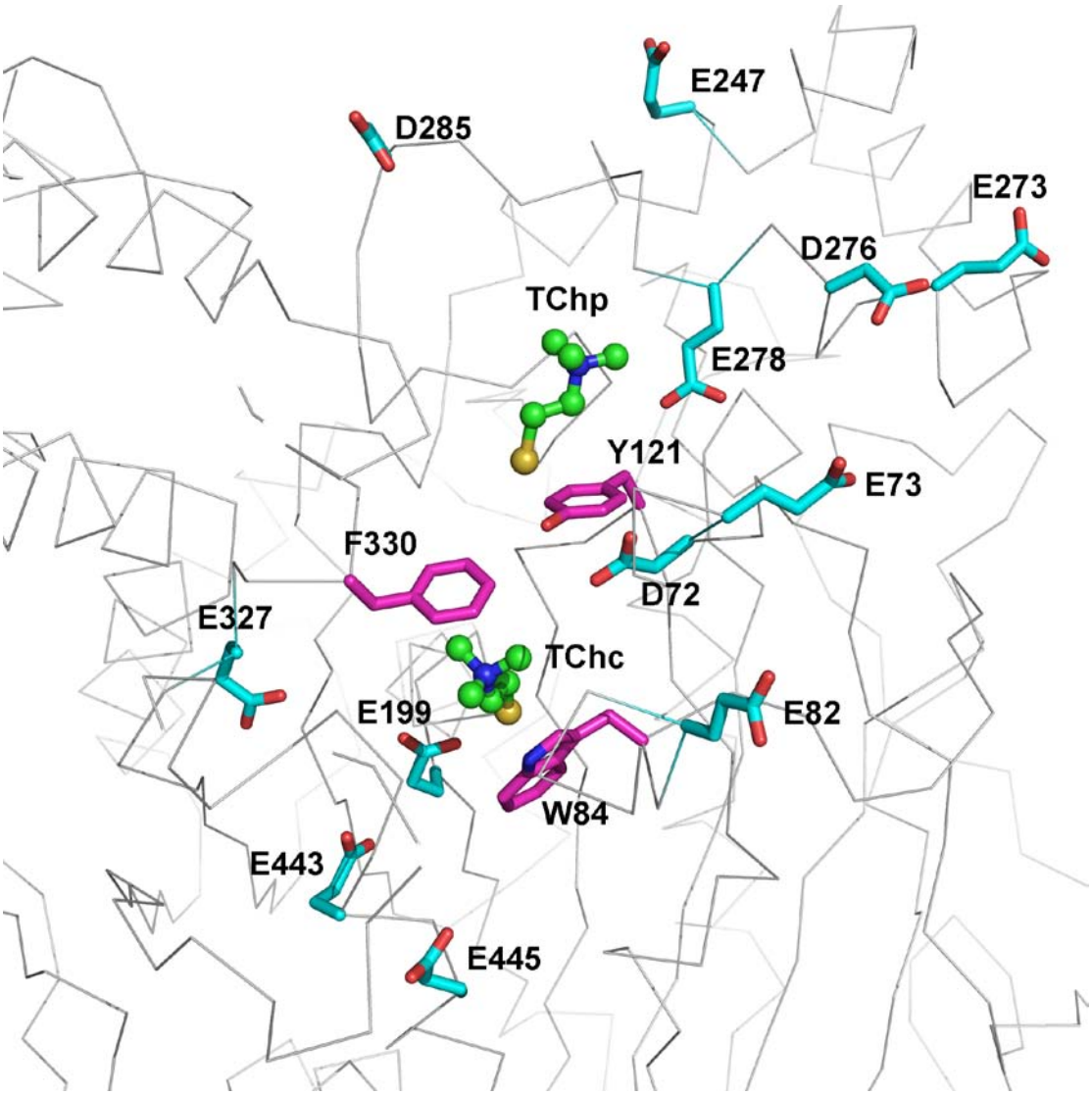

Figure S1 Interactions of TCh_C and TCh_P with acidic residues within the active-site gorge. A cross-section through the active-site gorge is displayed, showing acidic

residues as cyan stick models. The bottleneck aromatic residues, Y121 and F330, as well as W84, are shown as magenta sticks. TCh_C and TCh_P are displayed as green ball-and-stick models.

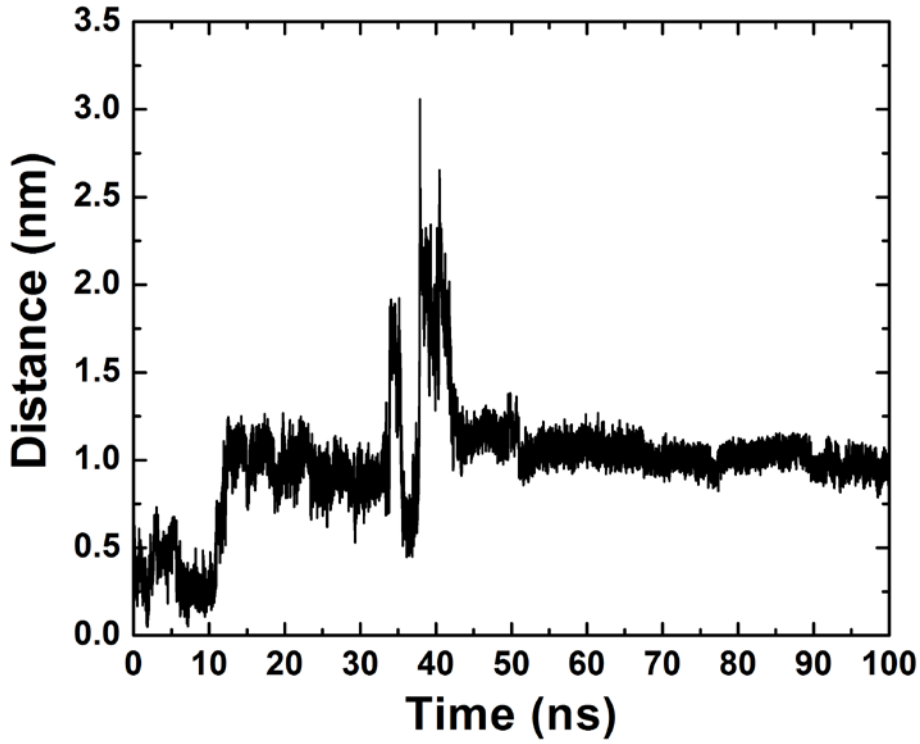

Figure S2 MD trajectory of 'mutated' TCh_P. In the trajectory shown, in both TCh_P and TCh_C the quaternary nitrogen atom has been replaced by a carbon, thus producing uncharged isosteric homologs.